Journal of Molecular Liquids 209 (2015) 738–744

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Abraham model correlations for solute transfer into 2-methoxyethanol from water and from the gas phase

Erin Hart [a], Damini Grover [a], Heidi Zettl [a], Victoria Koshevarova [a], Shoshana Zhang [a], Colleen Dai [a], William E. Acree Jr.[a,*], Igor A. Sedov [b], Mikhail A. Stolov [b], Michael H. Abraham [c]

[a] Department of Chemistry, University of North Texas, 1155 Union Circle Drive #305070, Denton, TX 76203, USA
[b] Department of Chemistry, Kazan Federal University, Kremlevskaya 18, Kazan 420008, Russia
[c] Department of Chemistry, University College London, 20 Gordon Street, London WC1H OAJ, UK

ARTICLE INFO

Article history:
Received 11 April 2015
Accepted 12 May 2015
Available online 25 June 2015

Keywords:
Partition coefficients
Infinite dilution activity coefficients
Solubility ratios
Hydrogen-bonding
Solute transfer
Headspace gas chromatographic method

ABSTRACT

Experimental solubilities have been determined for acenaphthene, biphenyl, benzoic acid, 3-nitrobenzoic acid, 4-nitrobenzoic acid, 2-methoxybenzoic acid, 4-methoxybenzoic acid, 3,4-dimethoxybenzoic acid, 4-aminobenzoic acid, 4-chlorobenzoic acid, 3,5-dinitro-2-methylbenzoic acid, 2-methylbenzoic acid, 3-methylbenzoic acid, 4-chloro-3-nitrobenzoic acid, 2-chloro-5-nitrobenzoic acid, 2-hydroxybenzoic acid, acetylsalicylic acid, 3,4-dichlorobenzoic acid, benzil, salicylamide, *trans*-stilbene, benzoin, and 9-fluorenone dissolved in 2-methoxyethanol at 298 K. Experimental infinite dilution activity coefficients and gas-to-liquid partition coefficients were measured for acetone, methanol, acetonitrile, butyl acetate, pyridine, 2-propanol, and dichloromethane in 2-methoxyethanol based a headspace gas chromatographic method. The measured solubility data, combined with published activity coefficients for several liquid organic solutes and solubility data for hydrogen gas, carbon dioxide, anthracene, pyrene, 2-nitrobenzoic acid, 2-chlorobenzoic acid, 3-chlorobenzoic acid, and 4-nitroaniline were used to derive Abraham model correlations for describing solute transfer into 2-methoxyethanol. The derived Abraham model correlations describe the experimental data to within 0.16 log units (or less).

1. Introduction

Organic solvents are used extensively in manufacturing processes involving chemical syntheses and purifications. Selection of an appropriate solvent for a given process requires knowledge of the solvent's physical properties and solubilizing abilities, as well as the solvent's toxicity, purchase price and disposal cost. Physical properties are largely governed by solvent–solvent interactions which are determined by molecular size and shape, and by the functional groups present in the solvent molecule. Solubilizing ability, on the other hand, depends more on the strength of the solute–solvent interactions relative to the strengths of both solvent–solvent and solute–solute interactions. Strong solute–solvent interactions tend to favor dissolution of the solute into the organic solvent media. Conversely weak solute–solvent interactions result in very low solute solubility.

During the past 50 years researchers have studied molecular interactions in fluid solutions using various spectroscopic, calorimetric and computational methods in hopes of achieving a better quantitative understanding of how these interactions affect chemical reaction rates and product yields, solute partitioning behavior between two completely immiscible (or partly miscible) phases, and solute solubility. The more successful of the proposed descriptive/predictive approaches include terms to represent contributions from both stronger interaction types (e.g., dipole–dipole and hydrogen-bonding) and weaker interaction types (dipole-induced dipole and nonspecific dispersion forces). Even in systems known to contain solute–solvent complexation and solvent/solute self-association the need to include weaker molecular interactions has been recognized. For example, Bertrand [1] showed that neglect of nonspecific molecular interactions can lead to significant errors in calculating thermodynamic association properties, particular in the case of weak molecular complexes, such as the chloroform–triethylamine complex.

The Abraham solvation parameter model [2–6] is one of the more successful approaches used in recent years to describe solute partitioning into and solute solubilities in organic solvent systems. Solute partitioning can be between two condensed phases (a biphasic aqueous-organic or organic–organic system):

$$\log(P \text{ or } C_{S,organic}/C_{S,water}) = c_p + e_p \cdot \mathbf{E} + s_p \cdot \mathbf{S} + a_p \cdot \mathbf{A} + b_p \cdot \mathbf{B} + v_p \cdot \mathbf{V} \quad (1)$$

* Corresponding author.
E-mail address: acree@unt.edu (W.E. Acree).

http://dx.doi.org/10.1016/j.molliq.2015.05.064
0167-7322/